

THE PHYSICAL BASIS FOR SPECTRAL VARIATIONS IN THERMAL INFRARED  
EMITTANCE OF SILICATES AND APPLICATION TO REMOTE SENSING

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The use of infrared spectroscopy for the remote characterization of planetary surfaces has received some attention due to efforts in the investigation of these bodies from space. In the 8 to 14 micron region, a depression in the emittance spectra of rocks (sometimes called reststrahlen) is related to the fundamental stretching vibrations of Si-O bonds and shifts in the location of this feature have been ascribed to variations in rock composition.

In 1952, Launer noted that the reststrahlen band shifted to shorter wavelengths as the Si:O ratio of the minerals he was examining increased and correlated the phenomenon with the change in silicate bonding from isolated tetrahedra through chains to framework structures.

The phenomenon he described can be interpreted as being due to the degree of polymerization of SiO<sub>4</sub> tetrahedra in silicate minerals. Framework silicates (e.g., quartz, feldspar) are highly polymerized with oxygen linking adjoining silicon cations. In the case of minerals having isolated tetrahedral structures (e.g., olivine), these bridges are broken by other cations (e.g., Mg, Fe). In crystallographic terms, this results in changes in the Si-O bond length and strength which, in turn, affects the location of the reststrahlen band. In 1969, Brown and Gibbs related bond length and strength to the average cation coordination of oxygen in silicate minerals. The oxygen coordination refers to the number of cations bonded to the oxygen anions. For example, the average oxygen coordination for various minerals is: quartz - 2.0; albite/orthoclase - 2.88; pyroxene - 3.33 and olivine - 4.0. They determined a linear relationship between the average coordination number, CN and Si-O, the mean Si-O bond distance:  $\text{Si-O} = 0.015 \text{ CN} + 1.579$  (units in Angstroms). This is the theoretical framework linking the spectral variations in the reststrahlen band and rock mineralogical composition.

Additional theoretical relationships, however, allow us to explore the significance of the spectral features with respect to silicate rock classification inasmuch as some schemes of classification are based, directly or indirectly, on the degree of polymerization of the silicate minerals. For example, the Differentiation Index of Thornton and Tuttle classifies igneous rocks on the basis of the amount of normative quartz, albite and orthoclase (all framework silicate and highly polymerized) relative to other mineral constituents with lower degrees of polymerization. A similar scheme relating silicate rock classification to chemical composition through the thermodynamic effects of polymerization has also been proposed.

Thus, it should be possible to investigate, quantify and model the relationships of reststrahlen spectral band location through silicate mineralogical composition to rock classification. As the Brown-Gibbs relationship is based on the averaged crystallographic properties of minerals,

it is useful for understanding their average thermal IR spectral response which can then be related to the location of the center of gravity of the emittance peaks. However, since in almost all silicates, not all of the oxygen ions are coordinated in the same way, there is a corresponding variation in the bond length and strength. The frequency distribution of the bond strengths is thus related to the spectral curve for a mineral. (This relationship has been used to gain insight into crystal structures as described in a rather large body of literature). Furthermore, the bond strength distribution, integrated over all the minerals in a rock, can next be related to the spectral curve for the whole sample.

It is planned to test these concepts, first through the use of laboratory-acquired data on the IR spectra and mineralogy of selected mineral and rock samples. As a suitable classification model is developed, it will be tested through overflights of appropriate rock outcrops using TIMS.